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INVARIANT IMBEDDING AND NEUTRON TRANSPORT
THEORY—V: DIFFUSION AS A LIMITING CASE

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SUMMARY

It is of interest for several reasons, from both the mathematical and physical points of view, to discuss in detail what happens to the various categories of transport equations derived from different applications of invariant imbedding as the velocity of the neutron is allowed to become arbitrarily large with a corresponding increase in the probability of a collision.

This idea is a quite natural one and one that has been pursued by a number of different investigators with different aims in mind. Diffusion theory classically has been regarded as an approximation to the more rigorous (but, of course, not completely rigorous) transport theory under the assumption of high velocity and small mean free path. Furthermore, passage to the limit in the "telegrapher's equation," a linear partial differential equation of hyperbolic type, has been carried out. We shall discuss one aspect of this below.

Our principal aim here is to study the limits of the non-linear functional equations obtained from the transport processes with finite velocity as the velocity increases without bound. In this way, we obtain corresponding results for heat or diffusion processes, where the physical picture is not as clear. Having obtained the equations in this indirect and complex fashion, we can then interpret them in such a way as to be able to derive them directly by invariant imbedding techniques. In all cases, the equations are of the generalized Riccati type which we recognize as characteristic of these processes of mathematical physics.

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INVARIANT IMBEDDING AND NEUTRON TRANSPORT THEORY—V:
DIFFUSION AS A LIMITING CASE

Richard Bellman
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G. Milton Wing

1. Introduction

In previous papers in this series, we have investigated a variety of simple models of transport theory by means of the functional equation technique of invariant imbedding. A number of references, together with some discussion of more complex versions will be found in [1].

Neutrons are mathematically abstracted to be point particles with finite velocities. Fission and scattering are characterized by certain probabilities of branching and reversal or reorientation of direction ("collision cross-sections") in the medium within which the process is occurring. In the great proportion of cases we assume no neutron-neutron interaction, although we have discussed this phenomenon in one paper, [8].

It is of interest for several reasons, from both the mathematical and physical points of view, to discuss in detail what happens to the various categories of transport equations derived from different applications of invariant imbedding as the velocity of the neutron is allowed to become arbitrarily large with a corresponding increase in the probability of a collision.

This idea is a quite natural one and one that has been

pursued by a number of different investigators with different aims in mind. Diffusion theory classically has been regarded as an approximation to the more rigorous (but, of course, not completely rigorous) transport theory under the assumption of high velocity and small mean free path, [2]. Furthermore, passage to the limit in the "telegrapher's equation," a linear partial differential equation of hyperbolic type, has been carried out. We shall discuss one aspect of this below.

From another direction, the discrete random walk process yields the diffusion equation in the limit. This observation has been made the basis for a considerable amount of analytic and computational effort, centering about the theme of "Monte Carlo" techniques.

Our principal aim here is to study the limits of the non-linear functional equations obtained from the transport processes with finite velocity as the velocity increases without bound. In this way, we obtain corresponding results for heat or diffusion processes, where the physical picture is not as clear. Having obtained the equations in this indirect and complex fashion, we can then interpret them in such a way as to be able to derive them directly by invariant imbedding techniques. In all cases, the equations are of the generalized Riccati type which we recognize as characteristic of these processes of mathematical physics.

At the present time, we are studying the question of treating Stefan-type diffusion problems by a similar passage to the limit in the equations derived from transport processes

with variable boundaries. This is, as might be expected, a complex problem. Some initial results are given in [9].

Throughout the paper, we use a simple generalization of the idealized one-dimensional rod process treated in [6]*. In the following section, we shall obtain some new equations for the flux within the rod, assuming finite velocities initially. In §3, we derive Fick's law for this simple process. This is important for our purposes, since it is the analysis of this result which suggests the combinations of functions which should be used in the limiting case. In §4, we study the limiting form of the internal flux as the velocity becomes infinite, and in §5 the diffusion process giving rise to the function obtained in this way is analyzed.

We then turn to the primary objective of this paper, the passage to the limit of the nonlinear integro-differential equation obtained for the reflected flux in the neutron transport case by means of the technique of invariant imbedding. In the concluding section, we show how to obtain the result by direct application of the imbedding technique to the diffusion process.

Throughout this paper, our methods are largely formal, since we are principally interested in demonstrating the applicability of invariance principles. The existence of relevant limits and the applicability of Laplace transform methods are taken for granted in order to arrive quickly at the desired equations. In the near future these questions will be studied in a rigorous fashion.

*See also [3,4,5].

For the simple mathematical models considered here, there is little difficulty in carrying out this program. Since, however, we know that the passage to the limit involves a reduction from a hyperbolic partial differential equation to a parabolic partial differential equation, involving inter alia a redundancy in the initial conditions, we can expect some difficulties in the general case. The corresponding study for ordinary differential equations when a limiting value of a parameter results in a drastic change in the order of the equation is of some subtlety. Particularly interesting examples of equations of this nature occur in various hydrodynamical investigations where viscosity plays the role of the parameter which approaches zero; cf. Wasow, [10].

2. The Transport Equation

To begin our work it is necessary to write down some transport equations in fairly general form. While some of them are not to be found in the literature, they may be readily derived by the methods of previous papers.

Consider a rod of material which transports neutrons, and let the neutrons have constant velocity c (monoenergetic case). The usual collision processes take place with the probability of a collision in a length Δ of the rod taken to be $\sigma\Delta + o(\Delta)$ where σ is a constant. On the average, $2k$ neutrons emerge from a collision inside the rod, k going to the left and k going to the right. We take the rod to extend from 0 to x (see Figure 1), and designate the

coordinate of an interior point by y .



To initiate the process, we suppose that there is a time dependent source, $q(t)$, neutrons incident to the left per second at x , and none at the end 0 . Finally, we suppose that particles emergent at 0 or x cannot re-enter the rod.

We write

(2.1) $u(y, t)$ = the average number of neutrons per second passing y at time t and moving to the right,

$v(y, t)$ = the average number of neutrons per second passing y at time t and moving to the left.

Using the methods outlined in [5], it is easily found that

$$(2.2) \quad \frac{\partial u}{\partial y} + \frac{1}{c} \frac{\partial u}{\partial t} = \sigma(k-1)u + \sigma v,$$

$$-\frac{\partial v}{\partial y} + \frac{1}{c} \frac{\partial v}{\partial t} = \sigma k u + \sigma(k-1)v,$$

$$u(0, t) = 0, \quad v(x, t) = q(t), \quad t \geq 0;$$

$$u(y, 0) = v(y, 0) = 0, \quad 0 \leq y < x.$$

For some purposes it is convenient to talk about the total flux from time 0 to t . We shall consistently use capital letters to indicate quantities integrated over time. Thus,

$$(2.3) \quad U(y,t) = \int_0^t u(y,z)dz,$$

$$Q(t) = \int_0^t q(z)dz,$$

etc. It is easy to see that the integrated quantities satisfy equations identical to (2.2) with the lower case letters being replaced by capitals.

Consider now the case in which the source consists of a single "trigger" neutron at $t = 0$. Thus, formally, $q(t) = \delta(t)$, where δ is the Dirac delta function. We focus attention on the particles reflected from the rod at x , writing $w(x,t)$ for the number emergent per second, and $W(x,t)$ for the total number emergent up to time t . Clearly,

$$(2.4) \quad u(x,t) \equiv w(x,t),$$

$$U(x,t) \equiv W(x,t).$$

However, it is well to regard the x in the arguments of w and W as referring to the length of the rod rather than to the coordinates of the end point of the rod. With this rather subtle distinction in mind one then finds, using the methods of [6],

$$(2.5) \quad \frac{\partial W}{\partial x} + \frac{2}{c} \frac{\partial W}{\partial t} = \sigma k + 2\sigma(k-1)W + \sigma k \int_0^t w(x,z)W(x,t-z)dz,$$

$$W(x,0) = W(0,t) = 0.$$

Notice that this characterizes the reflected flux in a fashion independent of the internal fluxes.

For the corresponding case in which there is a source $q(t)$, we write $F(x,t)$ for the reflected flux. Since the fundamental physical process is additive, as a consequence of our tacit assumption that there are no interactions between neutrons passing in opposite directions, we can write

$$(2.6) \quad F(x,t) = \int_0^t q(z)W(x,t-z)dz.$$

To find an equation satisfied by F , we utilize the Laplace transform, writing

$$(2.7) \quad F_L(x,s) = \int_0^\infty e^{-st}F(x,t)dt,$$

with a consistently similar notation for transforms of other functions. Then, from (2.5),

$$(2.8) \quad \frac{dW_L}{dx} + \frac{2}{c} sW_L = \frac{\partial k}{s} + 2\sigma(k-1)W_L + \sigma k s W_L^2,$$

$$W_L(0,s) = 0.$$

From (2.6),

$$(2.9) \quad F_L = q_L W_L.$$

Hence,

$$(2.10) \quad \frac{dF_L}{dx} + \frac{2}{c} sF_L = \frac{\partial k}{s} q_L + 2\sigma(k-1)F_L + \sigma k s F_L W_L,$$

which leads back to

$$(2.11) \quad \frac{\partial F}{\partial x} + \frac{2}{c} \frac{\partial F}{\partial t} = \sigma k Q(t) + 2\sigma(k-1)F(x,t) \\ + \sigma k \int_0^t w(x,z)F(x,t-z)dz,$$

$$F(0,t) = F(x,0) = 0.$$

This clearly reduces to (2.5) when $q(t) = \delta(t)$.

We shall derive one other special case of (2.11), corresponding to the case when $q(t) = 1$. While conceptually this is a bit harder to consider than the single trigger neutron case, it has the mathematical advantage of avoiding the δ -function. For this type of source we write the integrated flux as $R(x,t)$ and (2.11) becomes

$$(2.12) \quad \frac{\partial R}{\partial x} + \frac{2}{c} \frac{\partial R}{\partial t} = \sigma k t + 2\sigma(k-1)R(x,t) \\ + \sigma k \int_0^t w(x,z)R(x,t-z)dz.$$

But, from (2.6),

$$(2.13) \quad R(x,t) = \int_0^t w(x,t-z)dz.$$

Then we easily find

$$(2.14) \quad \frac{\partial R}{\partial x} + \frac{2}{c} \frac{\partial R}{\partial t} = \sigma k t + 2\sigma(k-1)R(x,t) \\ + \sigma k \int_0^t r(x,z)r(x,t-z)dz,$$

$$R(0,t) = R(x,0) = 0, \quad r(x,t) = \frac{\partial R}{\partial t}(x,t).$$

3. Pick's Law

If we subtract the second equation of (2.2) from the first we obtain

$$(3.1) \quad \frac{\partial}{\partial y}(u + v) + \frac{1}{c} \frac{\partial}{\partial t}(u - v) = -\sigma(u - v).$$

For large c one expects the second term on the left to be small. Hence we formally obtain the relation

$$(3.2) \quad \frac{\partial}{\partial y}(u + v) = -\sigma(u - v)$$

in the "limit of large velocity." Equation (3.2) is ordinarily referred to as Pick's Law, [2], which states that the net flux is proportional to the gradient of the concentration and in the opposite direction.

4. The Limiting Case Obtained from (2.2)

To obtain preliminary results we take Laplace transforms of (2.2). Thus, using the notation introduced in (2.7),

$$(4.1) \quad \begin{aligned} \frac{du_L}{dy} + \frac{s}{c} u_L &= \sigma(k-1)u_L + \sigma k v_L, \\ -\frac{dv_L}{dy} + \frac{s}{c} v_L &= \sigma k u_L + \sigma(k-1)v_L, \end{aligned}$$

$$u_L(0, s) = 0, \quad v_L(x, s) = q_L(s).$$

After rather extensive but rudimentary calculations we get

$$(4.2) \quad \begin{aligned} u_L(y, s) &= \frac{k\sigma q_L(s) \sinh \lambda y}{\left\{ \lambda \cosh \lambda x + \left(\frac{s}{c} + (1-k)\sigma \right) \sinh \lambda x \right\}}, \\ v_L(y, s) &= \frac{q_L(s) \left\{ \lambda \cosh \lambda y + \left(\frac{s}{c} + (1-k)\sigma \right) \sinh \lambda y \right\}}{\left\{ \lambda \cosh \lambda x + \left(\frac{s}{c} + (1-k)\sigma \right) \sinh \lambda x \right\}}, \end{aligned}$$

with

$$(4.3) \quad \lambda^2 = \left(\frac{s}{c}\right)^2 + \frac{2(1-k)\sigma}{c} s + \sigma^2(1-2k).$$

We now choose $k = 1/2$, which means physically that an average collision gives rise to one neutron. This choice eliminates the last term in (4.3). Since we seek a diffusion type equation, we let $c \rightarrow \infty$, i.e., the velocity become infinite. Clearly to preserve the process we must then require that $\sigma \rightarrow \infty$ in such a way that $\lim c/\sigma = D$, a constant. Hence, $\lim \lambda = \sqrt{s/D}$.

(It should be noted that a somewhat more general result could have been obtained by requiring, instead of $k = 1/2$, that $\lim \sigma^2(1-2k) = \alpha$. By so doing we could have accounted for cases of absorption or fission. To do this here would merely complicate the ensuing calculations.)

Bearing (3.2) in mind, we set

$$(4.4) \quad j_L(y, s) = \sigma(u_L(y, s) - v_L(y, s)),$$

$$j_{0,L}(y, s) = \lim_{\sigma \rightarrow \infty} j_L(y, s).$$

Let us consistently reserve the subscript zero to refer to quantities in the limit as $c \rightarrow \infty$.

We then discover that

$$(4.5) \quad j_{0,L}(y, s) = - \lim_{\sigma \rightarrow \infty} \frac{\sigma q_L(s) \lambda \cosh \lambda y}{\lambda \cosh \lambda x + \left(\frac{s}{c} + \frac{\sigma}{2}\right) \sinh \lambda x}$$

$$= - 2q_L(s) \frac{\sqrt{D^{-1}s} \cosh (y\sqrt{D^{-1}s})}{\sinh (x\sqrt{D^{-1}s})}.$$

5. A Classical Diffusion Problem

We now seek an ordinary diffusion problem which gives rise to the limiting expression found in (4.5). It is readily verified that if $\Theta(y,t)$ is implicitly determined by the relations

$$(5.1) \quad D \frac{\partial^2 \Theta}{\partial y^2} = \frac{\partial \Theta}{\partial t}, \quad \Theta(0,t) = 0, \quad \Theta(x,t) = 2q(t), \quad \Theta(y,0) = 0,$$

then, explicitly,

$$(5.2) \quad \Theta_L(y,s) = \frac{2q_L(s) \sinh(y\sqrt{D^{-1}s})}{\sinh(x\sqrt{D^{-1}s})},$$

and

$$(5.3) \quad \frac{d\Theta_L}{dy} = 2q_L(s) \sqrt{D^{-1}s} \frac{\cosh(y\sqrt{D^{-1}s})}{\sinh(x\sqrt{D^{-1}s})}.$$

We may summarize our results thus far as follows:

If we consider the transport problem formulated in (2.2) in the limiting case where $c \rightarrow \infty$, $c/\sigma \rightarrow D$, with $k = 1/2$, then the problem is formally equivalent to the classical diffusion problem (5.1). The quantity $\lim_{\sigma \rightarrow \infty} (u(y,t) + v(y,t))$ may be identified with $\Theta(y,t)$, while $\lim_{\sigma \rightarrow \infty} \sigma(u(y,t) - v(y,t))$ corresponds to $-\partial\Theta/\partial y$.

It is possible to identify $\Theta(y,t)$ with the total neutron flux (see [2]) although the diffusion may refer as well to heat or material concentration. The fact that a source of $2q(t)$ is required in the problem (5.1) may be rather puzzling until one notes from (4.2) that, formally, both $u(x,t)$ and $v(x,t)$ approach $q(t)$ as $c \rightarrow \infty$.

5. The Reflected Flux

Let us now turn to Equation (2.14) and try to carry out the same type of passage to the limit. It is clear that we must begin by investigating the quantity

$$(6.1) \quad H(x, t) = \sigma \{ R(x, t) - q(t) \},$$

which reduces to $\sigma \{ R(x, t) - t \}$, since $q(t) = 1$. Thus

$$(6.2) \quad R(x, t) = \frac{H(x, t)}{\sigma} + t,$$

$$r(x, t) = \frac{h(x, t)}{\sigma} + 1.$$

Substituting these in (2.14) with $k = 1/2$, we find

$$(6.3) \quad \frac{1}{\sigma} \frac{\partial H}{\partial x} + \frac{2}{c} \left(\frac{h}{\sigma} + 1 \right) = \frac{\sigma t}{2} - \sigma \left(\frac{H}{\sigma} + t \right) + \frac{\sigma}{2} \int_0^t \left\{ \frac{h(x, z)}{\sigma} + 1 \right\} \left\{ \frac{h(x, t-z)}{\sigma} + 1 \right\} dz.$$

From this we readily get

$$(6.4) \quad \frac{\partial H}{\partial x} + \frac{2\sigma}{c} \left(\frac{h}{\sigma} + 1 \right) = \frac{1}{2} \int_0^t h(x, z) h(x, t-z) dz,$$

$$H(x, 0) = 0, \quad H(0, t) = -\sigma t.$$

Passing to the limit as in §5 we get (at least formally)

$$(6.5) \quad \frac{\partial H_0}{\partial x} + 2D^{-1} = \frac{1}{2} \int_0^t h_0(x, z) h_0(x, t-z) dz,$$

$$H_0(x, 0) = 0, \quad H_0(0, t) = -\infty;$$

where $H_0(x,t) = \lim_{\sigma \rightarrow \infty} H(x,t)$, etc., as agreed. That (6.5) is the correct limiting form may be established by a Laplace transform argument similar to that of the last section. We omit the details.

It is of some interest to evaluate H_0 . This may be done by solving (6.5), of course. However, it is easier for us to note from (4.5) that

$$(6.6) \quad h_{0,L}(x,s) = -2q_L(s) \frac{\sqrt{D^{-1}s} \cosh(x\sqrt{D^{-1}s})}{\sinh(x\sqrt{D^{-1}s})} \\ = -\frac{2}{\sqrt{SD}} \coth(x\sqrt{D^{-1}s}),$$

since $q(t) = 1$. We find

$$(6.7) \quad h_0(x,t) = -\frac{2}{\sqrt{\pi t D}} \left\{ 1 + 2 \sum_{n=1}^{\infty} e^{-\frac{x^2 n^2}{t D}} \right\} \\ = -\frac{2}{x} \theta_0\left(\frac{1}{2}, \frac{t}{Dx^2}\right),$$

where θ_0 is a theta function.

The analogue of (6.5) may be derived easily for the case in which there is an arbitrary source $Q(t)$. The result is

$$(6.8) \quad \frac{\partial J_0}{\partial x} + 2D^{-1}q(t) = \frac{1}{2} \int_0^t h_0(x,z) J_0(x,t-z) dz,$$

$$J_0(x,0) = 0, \quad J_0(0,t) = -\infty,$$

$$J_0(x,t) = \lim_{\sigma \rightarrow \infty} \sigma \{F(x,t) - Q(t)\},$$

where F is as in (2.6).

We now readily see the following result:

If we consider the transport problem formulated in (2.2) in the limiting case then the quantity $J_0(x,t)$ is formally equivalent to the quantity $-\frac{\partial}{\partial y} \int_0^t \theta(y,z) dz \Big|_{y=x}$ where θ is defined by (5.1). Further J_0 satisfies (6.8) with $h_0(x,t)$ given by (6.5).

7. A Direct Invariant Imbedding Approach in Diffusion Theory

The equations thus far obtained are not new, though our approach to them may be somewhat novel. To conclude our work here we shall present a method of obtaining (6.8) by invariant imbedding techniques without venturing outside the confines of ordinary diffusion theory. The method described holds promise of being applicable in much more complicated diffusion processes than that described here, and, in particular, may eventually yield new formulations of Stefan-type problems.

To be consistent in our viewpoint, we now think of $\phi(y,t)$ as the density of neutrons at y at time t . Then the net neutron current density $c(y,t)$ is provided by Fick's Law, in the ordinary diffusion approach [2],

$$(7.1) \quad c(y,t) = -D \frac{\partial}{\partial y} \phi(y,t).$$

The conservation of particles (since there is no internal production) requires in any interval (a,b) of the rod

$$(7.2) \quad c(b,t) - c(a,t) = -\frac{\partial}{\partial t} \int_a^b \phi(y,t) dy.$$

Let us write, for the net current emerging from our rod of length x , $k(x,t)$. Here, again, while it is true that $k(x,t) = c(x,t)$ we choose to regard the x in the function k as referring to the length of the rod. Thus $k(x + \Delta, t)$ is the net current emergent from a rod of length $x + \Delta$, source $2q(t)$ at $(x + \Delta)$, other initial and boundary conditions being as before.

We now try to express $k(x + \Delta, t)$ in terms of $k(x, t)$. Applying (7.2) to the rod of length $x + \Delta$ we find

$$(7.3) \quad k(x + \Delta, t) - c(x, t) = - \frac{\partial}{\partial t} \int_x^{x+\Delta} \phi(y, t) dy,$$

or, integrating over time,

$$(7.4) \quad K(x + \Delta, t) - C(x, t) = - \int_x^{x+\Delta} \phi(y, t) dy.$$

We now seek expressions for $C(x, t)$ and ϕ . To find $C(x, t)$ we note that we have thus far disregarded the part of the rod from 0 to x . By the continuity conditions imposed by diffusion theory, we know that $C(x, t)$ is merely the current out of x due to the source $\phi(x, t)$ imposed. Let us suppose that a steady source of unit strength produces a current out of the rod of $p(x, t)$. Then a source $\phi(x, t)$ will produce an integrated current

$$(7.5) \quad C(x, t) = \int_0^t p(x, t - z) \phi(x, z) dz.$$

(This is just Duhamel's Principle [7]).

As yet we have not used (7.1). From it we find

$$(7.6) \quad \phi(x, t) = \frac{\Delta}{D} k(x + \Delta, t) + 2q(t) + o(\Delta).$$

Substituting (7.5) and (7.6) in (7.4), we obtain

$$(7.7) \quad K(x + \Delta, t) = \int_0^t p(x, t - z) \left\{ \frac{\Delta}{D} k(x + \Delta, z) + 2q(z) \right\} dz \\ - 2\Delta q(t) + o(\Delta).$$

But, by Duhamel's Principle,

$$(7.8) \quad \int_0^t p(x, t - z) 2q(z) dz = K(x, t).$$

Thus

$$(7.9) \quad \frac{\partial K}{\partial x} + 2q(t) = \frac{1}{D} \int_0^t p(x, t - z) k(x, z) dz.$$

This agrees with (6.8) upon identifying k with Dj_0 and p with $\frac{D}{2} h_0$, the factor $1/2$ occurring because p is the current due to a unit source, while h_0 is obtained from a source of strength 2.

It is clear that

$$(7.10) \quad K(x, 0) = 0.$$

To find $K(0, t)$ we note from (7.6) that

$$\phi(0, t) = 0 = \frac{\Delta}{D} k(\Delta, t) + 2q(t) + o(\Delta),$$

so that for $q(t) > 0$,

$$(1.11) \quad K(0, t) = -\infty.$$

Clearly, in case $q = 1$, we have

$$(1.12) \quad \frac{\partial F}{\partial x} + 2 = \frac{1}{D} \int_0^t p(x, t-z)p(x, z)dz,$$

$$F(x, 0) = 0, \quad F(0, t) = -\infty.$$

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